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# 2-Chloro-6-(2,3-dichlorobenzenesulfonamido)benzoic acid

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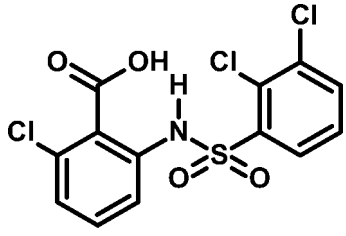
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.038; $wR$ factor = 0.104; data-to-parameter ratio = 15.0.

In the title compound, $C_{13}H_8Cl_3NO_4S$, the aromatic rings are oriented at a dihedral angle of 68.94 (1)° and the molecule adopts a V-shape. An intramolecular N—H···O interaction generates a six-membered $S(6)$ ring motif. In the crystal, pairs of O—H···O hydrogen bonds involving the carboxy group link the molecules into inversion dimers with an $R_2^2(8)$ motif. N—H···O and non-classical C—H···O interactions connect the molecules, forming sheets propagating in (100).

## Related literature

For the synthesis, see: Arshad *et al.* (2012) For related structures, see: Arshad *et al.* (2009, 2011). For graph-set notation, see: Bernstein *et al.* (1995).



## Experimental

### Crystal data

$C_{13}H_8Cl_3NO_4S$
$M_r$ = 380.61
Monoclinic, $P2_1/c$
$a$ = 9.0164 (3) Å
$b$ = 18.6017 (5) Å
$c$ = 9.8574 (3) Å
$\beta$ = 111.653 (3)°
$V$ = 1536.62 (8) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 6.83 mm$^{-1}$
$T$ = 296 K
0.38 × 0.20 × 0.18 mm

### Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas, CCD) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min}$ = 0.467, $T_{max}$ = 1.000
11742 measured reflections
3018 independent reflections
2597 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.104
$S$ = 1.04
3018 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.60 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O3 | 0.86 | 2.55 | 2.940 (2) | 108 |
| C12—H12···O3$^{i}$ | 0.93 | 2.59 | 3.425 (3) | 150 |
| O3—H3···O4$^{ii}$ | 0.82 | 1.85 | 2.666 (2) | 176 |
| N1—H1···O2$^{iii}$ | 0.86 | 2.30 | 3.128 (2) | 162 |
| C5—H5···O4$^{iv}$ | 0.93 | 2.53 | 3.256 (4) | 135 |
| C10—H10···O1$^{v}$ | 0.93 | 2.51 | 3.165 (3) | 127 |

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x+1, -y+1, -z+2$; (iii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iv) $-x+1, -y+1, -z+1$; (v) $x+1, y, z$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *X-SEED* (Barbour, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5312).

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# supplementary materials

*Acta Cryst.* (2013). E**69**, o832 [doi:10.1107/S1600536813011574]

## 2-Chloro-6-(2,3-dichlorobenzenesulfonamido)benzoic acid

**Ayesha Munir, Hafiz Mubashar-ur-Rehman, Abdullah M. Asiri, Islam Ullah Khan and Muhammad Nadeem Arshad**

### Comment

In connection to synthesis of halogenated sulfonamide derivatives 2-Chloro-4-(2-iodobenzenesulfonamido)benzoic acid (Arshad *et al.*, 2011) and 2-Chloro-5-(2-iodobenzenesulfonamido)benzoic acid (Arshad *et al.*, 2009), we are reporting the crystal structure of title compound.

The two aromatic rings [(C1—C6) & (C7—C12)] in the structure of molecule are oriented at dihedral angle of 68.94 (1)°. The carboxylic group (C13/O3/O4) is twisted at 58.11 (1)° with respect to its mother aromatic ring (C7—C12) and its atoms C13, O3 & O4 are away by -0.1938 (35)Å , 0.6924 (39)Å , -1.1739 (39)Å repectively from the mean plane generating from atoms C7/C8/C9/C10/C11/C12 with the r.m.s deviation of 0.0183 (15) Å. The amino and carboxylic groups are involved in classical N1—H1···O3 intramolecular hydrogen bonding interaction and produce six membered ring motif $S^1_1$ (6) (Bernstein *et al.* 1995) which is oriented at dihedral angles of 54.30 (11)° & 18.98 (12)° with respect to two aromatic rings [(C1—C6) & (C7—C12)], respectively. On the other hand the amino group get connected with oxygen of $SO_2$ to form intermolecular N1—H1···O2 hydrogen bond. The carboxylic group gives typical inversion dimerization by generating eight membered ring motif $R^2_2$ (8) (Bernstein *et al.* 1995) through O3—H3···O4 interaction. The non-clasical C—H···O type interaction have also been observed in the molecule (Fig. 2) for which symmetry detail are available in Table 1.

### Experimental

The title compound was synthesised following the literature method (Arshad *et al.*, 2012) and recrystallized from ethyl-acetate under slow evaporation at room temperature.

### Refinement

All the H-atoms were positioned with idealized geometry with C—H = 0.93 Å, N—H = 0.86 Å, O—H = 0.82 Å and were refined as riding with $U_{iso}$(H) = 1.2 $U_{eq}$(K), where K = C, N & O for all H-atoms. The reflections (0 1 2), (1 3 1), (1 0 0), (2 1 0) & (0 2 0) are omitted in final refinement.

### Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *X-SEED* (Barbour, 2001).

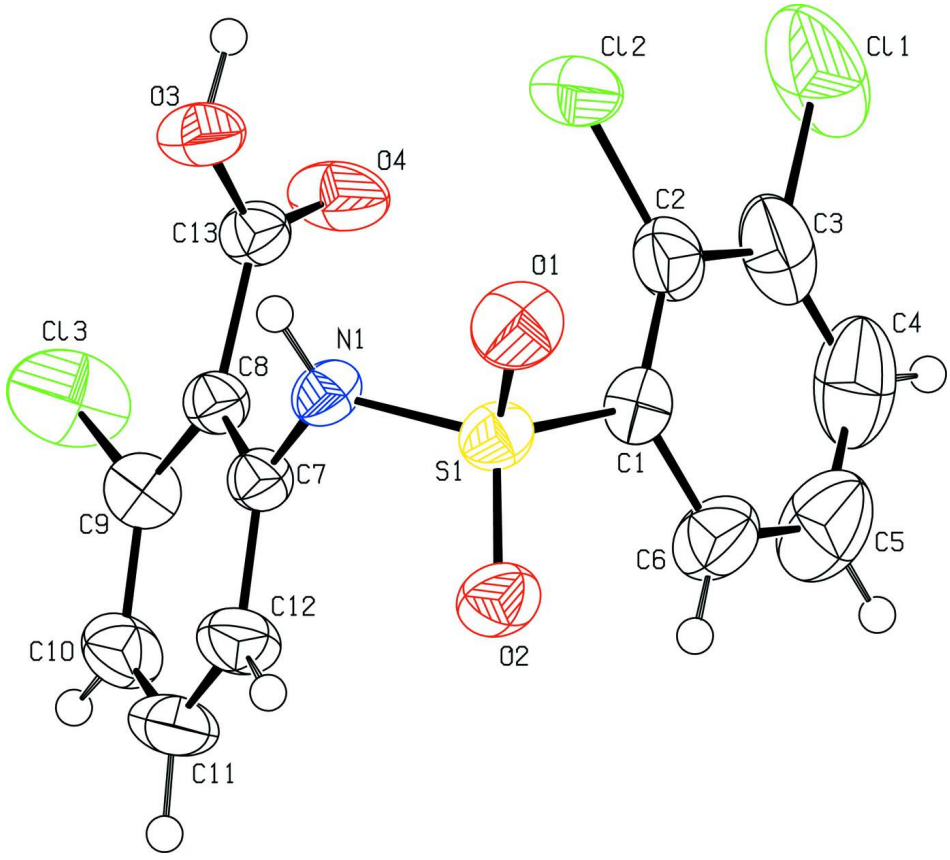


**Figure 1**

The labelled structure of ($C_{13}$ $H_8$ $Cl_3$ N $O_4$ S) with 50% probability of thermal ellipsoids.

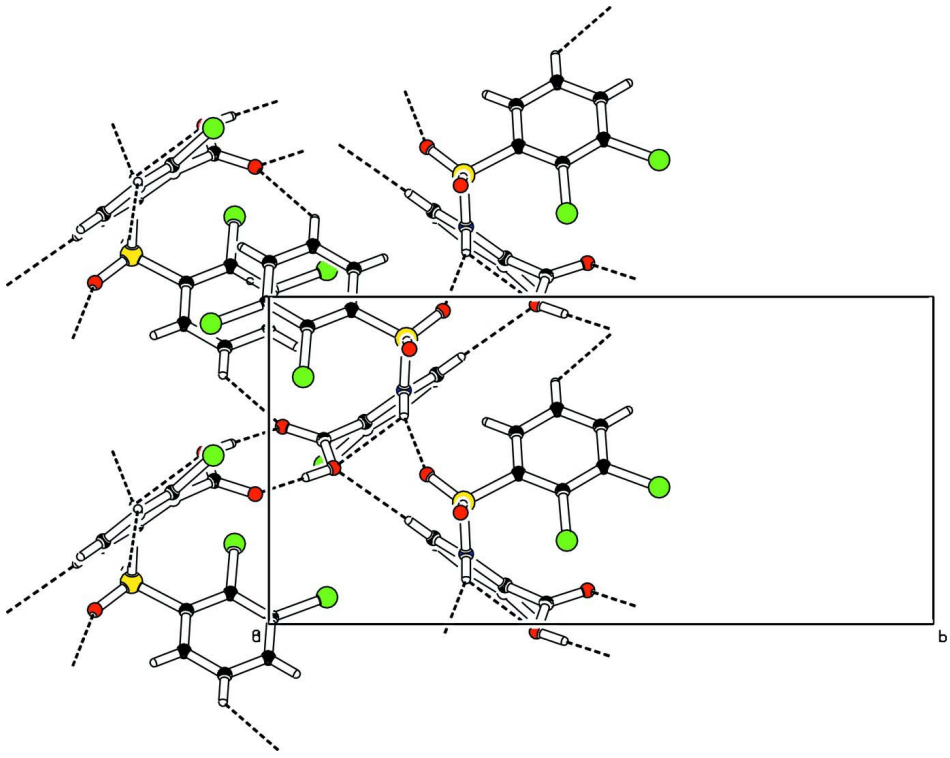


**Figure 2**

A perspective view showing two dimensional network generating through O—H···O, N—H···O and C—H···O hydrogen bonds, drawn using dashed lines.

### 2-Chloro-6-(2,3-dichlorobenzenesulfonamido)benzoic acid

*Crystal data*

$C_{13}H_8Cl_3NO_4S$
$M_r$ = 380.61
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 9.0164 (3) Å
$b$ = 18.6017 (5) Å
$c$ = 9.8574 (3) Å
$\beta$ = 111.653 (3)°
$V$ = 1536.62 (8) Å$^3$
$Z$ = 4
$F(000)$ = 768
$D_x$ = 1.645 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54184 Å
Cell parameters from 5339 reflections
$\theta$ = 4.8–73.0°
$\mu$ = 6.83 mm$^{-1}$
$T$ = 296 K
Prismatic, colorless
0.38 × 0.20 × 0.18 mm

*Data collection*

Agilent SuperNova (Dual, Cu at zero, Atlas, CCD) diffractometer
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min}$ = 0.467, $T_{max}$ = 1.000
11742 measured reflections
3018 independent reflections
2597 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025
$\theta_{max}$ = 73.1°, $\theta_{min}$ = 5.4°
$h$ = −10→11
$k$ = −22→22
$l$ = −12→11

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.104$
$S = 1.04$
3018 reflections
201 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 1.0131P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.55$ e Å$^{-3}$
$\Delta\rho_{min} = -0.60$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0022 (2)

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.21203 (15) | 0.41272 (5) | 0.58195 (14) | 0.1161 (5) |
| Cl2 | 0.17428 (9) | 0.55156 (5) | 0.74492 (8) | 0.0718 (3) |
| Cl3 | 0.94473 (9) | 0.58369 (5) | 1.01517 (11) | 0.0797 (3) |
| S1 | 0.24536 (6) | 0.70690 (3) | 0.62789 (6) | 0.03763 (17) |
| O1 | 0.1045 (2) | 0.71147 (11) | 0.6596 (2) | 0.0562 (5) |
| O2 | 0.2792 (2) | 0.76184 (9) | 0.54279 (18) | 0.0482 (4) |
| O3 | 0.5137 (2) | 0.59728 (8) | 1.02304 (19) | 0.0460 (4) |
| H3 | 0.4816 | 0.5600 | 1.0473 | 0.055* |
| O4 | 0.6012 (2) | 0.52066 (9) | 0.8971 (2) | 0.0572 (5) |
| N1 | 0.3928 (2) | 0.70318 (10) | 0.78616 (19) | 0.0357 (4) |
| H1 | 0.3706 | 0.7032 | 0.8638 | 0.043* |
| C1 | 0.2524 (3) | 0.62421 (13) | 0.5405 (2) | 0.0417 (5) |
| C2 | 0.2255 (3) | 0.55805 (14) | 0.5932 (3) | 0.0510 (6) |
| C3 | 0.2403 (4) | 0.49629 (16) | 0.5195 (4) | 0.0693 (9) |
| C4 | 0.2779 (4) | 0.5009 (2) | 0.3962 (4) | 0.0843 (11) |
| H4 | 0.2867 | 0.4592 | 0.3476 | 0.101* |
| C5 | 0.3022 (5) | 0.5663 (2) | 0.3450 (4) | 0.0804 (10) |
| H5 | 0.3269 | 0.5691 | 0.2615 | 0.096* |
| C6 | 0.2903 (4) | 0.62797 (17) | 0.4168 (3) | 0.0583 (7) |
| H6 | 0.3078 | 0.6724 | 0.3823 | 0.070* |
| C7 | 0.5563 (2) | 0.69989 (11) | 0.8019 (2) | 0.0327 (4) |
| C8 | 0.6539 (2) | 0.64427 (11) | 0.8821 (2) | 0.0329 (4) |
| C9 | 0.8156 (3) | 0.64584 (13) | 0.9024 (3) | 0.0418 (5) |
| C10 | 0.8775 (3) | 0.69735 (14) | 0.8382 (3) | 0.0485 (6) |

| | | | | |
|---|---|---|---|---|
| H10 | 0.9852 | 0.6970 | 0.8518 | 0.058* |
| C11 | 0.7777 (3) | 0.74919 (15) | 0.7535 (3) | 0.0536 (7) |
| H11 | 0.8175 | 0.7829 | 0.7061 | 0.064* |
| C12 | 0.6188 (3) | 0.75223 (13) | 0.7376 (3) | 0.0467 (6) |
| H12 | 0.5540 | 0.7892 | 0.6840 | 0.056* |
| C13 | 0.5870 (3) | 0.58240 (11) | 0.9374 (2) | 0.0348 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.1280 (9) | 0.0446 (5) | 0.1266 (9) | −0.0192 (5) | −0.0106 (7) | 0.0082 (5) |
| Cl2 | 0.0734 (5) | 0.0782 (5) | 0.0597 (4) | −0.0271 (4) | 0.0197 (3) | 0.0177 (4) |
| Cl3 | 0.0502 (4) | 0.0720 (5) | 0.1115 (7) | 0.0207 (3) | 0.0236 (4) | 0.0361 (5) |
| S1 | 0.0363 (3) | 0.0420 (3) | 0.0365 (3) | 0.0046 (2) | 0.0158 (2) | 0.0039 (2) |
| O1 | 0.0388 (9) | 0.0760 (13) | 0.0587 (11) | 0.0094 (8) | 0.0238 (8) | 0.0034 (9) |
| O2 | 0.0531 (9) | 0.0456 (10) | 0.0438 (9) | 0.0048 (7) | 0.0153 (7) | 0.0123 (7) |
| O3 | 0.0692 (11) | 0.0324 (8) | 0.0514 (10) | −0.0026 (8) | 0.0397 (9) | 0.0004 (7) |
| O4 | 0.0914 (14) | 0.0287 (8) | 0.0748 (13) | −0.0047 (8) | 0.0580 (11) | −0.0055 (8) |
| N1 | 0.0380 (9) | 0.0422 (10) | 0.0303 (9) | 0.0018 (7) | 0.0167 (7) | 0.0005 (7) |
| C1 | 0.0419 (11) | 0.0449 (13) | 0.0356 (11) | −0.0006 (10) | 0.0111 (9) | −0.0023 (9) |
| C2 | 0.0446 (13) | 0.0496 (15) | 0.0468 (14) | −0.0081 (11) | 0.0027 (11) | 0.0017 (11) |
| C3 | 0.0639 (17) | 0.0444 (16) | 0.072 (2) | −0.0044 (13) | −0.0075 (15) | −0.0037 (14) |
| C4 | 0.095 (2) | 0.070 (2) | 0.070 (2) | 0.0129 (19) | 0.0098 (19) | −0.0296 (18) |
| C5 | 0.108 (3) | 0.078 (2) | 0.0594 (19) | 0.012 (2) | 0.0362 (19) | −0.0156 (17) |
| C6 | 0.0753 (18) | 0.0590 (17) | 0.0460 (14) | 0.0016 (14) | 0.0285 (13) | −0.0020 (12) |
| C7 | 0.0369 (10) | 0.0302 (10) | 0.0325 (10) | −0.0020 (8) | 0.0148 (8) | −0.0012 (8) |
| C8 | 0.0405 (10) | 0.0270 (10) | 0.0336 (10) | −0.0026 (8) | 0.0166 (8) | −0.0021 (8) |
| C9 | 0.0396 (11) | 0.0391 (12) | 0.0474 (13) | 0.0024 (9) | 0.0168 (10) | 0.0002 (10) |
| C10 | 0.0369 (11) | 0.0556 (15) | 0.0568 (15) | −0.0089 (10) | 0.0218 (11) | −0.0030 (12) |
| C11 | 0.0518 (14) | 0.0530 (16) | 0.0602 (16) | −0.0145 (11) | 0.0257 (12) | 0.0121 (12) |
| C12 | 0.0468 (13) | 0.0401 (13) | 0.0515 (14) | −0.0042 (10) | 0.0161 (11) | 0.0126 (10) |
| C13 | 0.0418 (11) | 0.0297 (10) | 0.0357 (11) | 0.0013 (8) | 0.0174 (9) | 0.0012 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C3 | 1.725 (3) | C4—C5 | 1.366 (5) |
| Cl2—C2 | 1.725 (3) | C4—H4 | 0.9300 |
| Cl3—C9 | 1.724 (2) | C5—C6 | 1.373 (4) |
| S1—O1 | 1.4179 (17) | C5—H5 | 0.9300 |
| S1—O2 | 1.4247 (17) | C6—H6 | 0.9300 |
| S1—N1 | 1.6357 (18) | C7—C12 | 1.389 (3) |
| S1—C1 | 1.776 (2) | C7—C8 | 1.399 (3) |
| O3—C13 | 1.279 (3) | C8—C9 | 1.397 (3) |
| O3—H3 | 0.8200 | C8—C13 | 1.493 (3) |
| O4—C13 | 1.238 (3) | C9—C10 | 1.375 (3) |
| N1—C7 | 1.426 (3) | C10—C11 | 1.372 (4) |
| N1—H1 | 0.8600 | C10—H10 | 0.9300 |
| C1—C6 | 1.384 (3) | C11—C12 | 1.383 (3) |
| C1—C2 | 1.391 (3) | C11—H11 | 0.9300 |
| C2—C3 | 1.391 (4) | C12—H12 | 0.9300 |

| | | | |
|---|---|---|---|
| C3—C4 | 1.380 (5) | | |
| | | | |
| O1—S1—O2 | 119.37 (11) | C5—C6—C1 | 120.3 (3) |
| O1—S1—N1 | 105.73 (10) | C5—C6—H6 | 119.9 |
| O2—S1—N1 | 108.47 (10) | C1—C6—H6 | 119.9 |
| O1—S1—C1 | 110.74 (12) | C12—C7—C8 | 120.0 (2) |
| O2—S1—C1 | 106.38 (11) | C12—C7—N1 | 119.82 (19) |
| N1—S1—C1 | 105.32 (10) | C8—C7—N1 | 120.19 (18) |
| C13—O3—H3 | 109.5 | C9—C8—C7 | 118.12 (19) |
| C7—N1—S1 | 123.33 (14) | C9—C8—C13 | 120.35 (19) |
| C7—N1—H1 | 118.3 | C7—C8—C13 | 121.44 (18) |
| S1—N1—H1 | 118.3 | C10—C9—C8 | 121.9 (2) |
| C6—C1—C2 | 120.5 (2) | C10—C9—Cl3 | 118.17 (18) |
| C6—C1—S1 | 116.6 (2) | C8—C9—Cl3 | 119.94 (18) |
| C2—C1—S1 | 122.88 (19) | C11—C10—C9 | 118.9 (2) |
| C1—C2—C3 | 118.2 (3) | C11—C10—H10 | 120.5 |
| C1—C2—Cl2 | 121.7 (2) | C9—C10—H10 | 120.5 |
| C3—C2—Cl2 | 120.2 (2) | C10—C11—C12 | 121.2 (2) |
| C4—C3—C2 | 120.7 (3) | C10—C11—H11 | 119.4 |
| C4—C3—Cl1 | 119.1 (3) | C12—C11—H11 | 119.4 |
| C2—C3—Cl1 | 120.2 (3) | C11—C12—C7 | 119.8 (2) |
| C5—C4—C3 | 120.4 (3) | C11—C12—H12 | 120.1 |
| C5—C4—H4 | 119.8 | C7—C12—H12 | 120.1 |
| C3—C4—H4 | 119.8 | O4—C13—O3 | 123.6 (2) |
| C4—C5—C6 | 120.0 (3) | O4—C13—C8 | 119.58 (19) |
| C4—C5—H5 | 120.0 | O3—C13—C8 | 116.82 (18) |
| C6—C5—H5 | 120.0 | | |
| | | | |
| O1—S1—N1—C7 | −178.47 (17) | S1—C1—C6—C5 | 178.3 (3) |
| O2—S1—N1—C7 | −49.3 (2) | S1—N1—C7—C12 | 55.1 (3) |
| C1—S1—N1—C7 | 64.24 (19) | S1—N1—C7—C8 | −125.01 (19) |
| O1—S1—C1—C6 | 132.5 (2) | C12—C7—C8—C9 | 3.9 (3) |
| O2—S1—C1—C6 | 1.4 (2) | N1—C7—C8—C9 | −175.94 (19) |
| N1—S1—C1—C6 | −113.6 (2) | C12—C7—C8—C13 | −172.5 (2) |
| O1—S1—C1—C2 | −49.0 (2) | N1—C7—C8—C13 | 7.6 (3) |
| O2—S1—C1—C2 | 179.83 (19) | C7—C8—C9—C10 | −4.4 (3) |
| N1—S1—C1—C2 | 64.8 (2) | C13—C8—C9—C10 | 172.1 (2) |
| C6—C1—C2—C3 | 1.0 (4) | C7—C8—C9—Cl3 | 173.60 (17) |
| S1—C1—C2—C3 | −177.45 (19) | C13—C8—C9—Cl3 | −9.9 (3) |
| C6—C1—C2—Cl2 | −178.7 (2) | C8—C9—C10—C11 | 1.0 (4) |
| S1—C1—C2—Cl2 | 2.9 (3) | Cl3—C9—C10—C11 | −177.0 (2) |
| C1—C2—C3—C4 | −1.1 (4) | C9—C10—C11—C12 | 3.0 (4) |
| Cl2—C2—C3—C4 | 178.6 (2) | C10—C11—C12—C7 | −3.4 (4) |
| C1—C2—C3—Cl1 | 178.77 (19) | C8—C7—C12—C11 | −0.2 (4) |
| Cl2—C2—C3—Cl1 | −1.5 (3) | N1—C7—C12—C11 | 179.7 (2) |
| C2—C3—C4—C5 | 0.4 (5) | C9—C8—C13—O4 | −56.9 (3) |
| Cl1—C3—C4—C5 | −179.4 (3) | C7—C8—C13—O4 | 119.5 (2) |
| C3—C4—C5—C6 | 0.4 (6) | C9—C8—C13—O3 | 124.7 (2) |
| C4—C5—C6—C1 | −0.5 (5) | C7—C8—C13—O3 | −58.9 (3) |

| | |
|---|---|
| C2—C1—C6—C5 | −0.2 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O3 | 0.86 | 2.55 | 2.940 (2) | 108 |
| C12—H12···O3$^{i}$ | 0.93 | 2.59 | 3.425 (3) | 150 |
| O3—H3···O4$^{ii}$ | 0.82 | 1.85 | 2.666 (2) | 176 |
| N1—H1···O2$^{iii}$ | 0.86 | 2.30 | 3.128 (2) | 162 |
| C5—H5···O4$^{iv}$ | 0.93 | 2.53 | 3.256 (4) | 135 |
| C10—H10···O1$^{v}$ | 0.93 | 2.51 | 3.165 (3) | 127 |

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2; (ii) −*x*+1, −*y*+1, −*z*+2; (iii) *x*, −*y*+3/2, *z*+1/2; (iv) −*x*+1, −*y*+1, −*z*+1; (v) *x*+1, *y*, *z*.